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Commentary

Modes of Microscopy*

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Before automation can be contemplated, one must define the problem completely. Included in this simple but fundamental query are the questions: What are we looking for? What other background material is there? What sensitivity is needed? What are the sizes of the particles in question? The last question relates to the degree of uncertainty involved. As the particle size gets smaller, the information that can be obtained about it gets less.

The general techniques available to us include: optical microscopy, transmission electron microscopy (TEM), scanning electron microscopy (SEM) which can also be used as an electron probe, and x-ray diffraction. Of these, optical microscopy relates only to large particles. Different techniques are applicable, depending on the characteristic under discussion and the size of the sample, as indicated by Table 1.

Table 1. Investigation techniques.

Characteristic	Technique	
	Bulk sample	Minute sample
Composition	Chemistry	Microprobe
Structure	X-ray diffraction	Electron diffraction
Morphology	—	Electron microscopy

TEM, as conventionally used, presents certain problems. First is the variable appearance of the mineral in question; second, the lack of sufficiently specific information for the development of a "complete pattern recognition," which is essential if the data are to be automated. With the SEM, however, the pattern recognition problem can be simplified. Probable decision algorithms are available which enable one to make reasonable classifications and distinctions of particles based on the microchemical information obtained.

Several techniques for automation exist today. Automated x-ray diffractometry is available, but is not really suited to the identification of material particle by particle. The SEM with probe capability and automatically controlled x-ray spectrometers permit particle counting and sizing and some microchemical analysis. In Eugene White's system a certain number of preset energies permit him to look at five or six elements at one time. Beam writing under computer control is quite common, and some of the work done at Mt. Sinai has indicated that it is possible to parametrize automatically the x-ray information from a SEM microprobe with energy dispersive detectors.

There are certain problems with the SEM–microprobe analytical system. First is the possibility of contamination of the x-ray spectra with x-rays generated by backscattered electrons. Another is that different minerals may have similar chemistries. If the sample is not sufficiently dispersed, particles may overlap. The spatial resolution of the system that I use is only 250 Å . Finally, there is the problem of time constraint. If you can confine your problem, for example by dealing only with fibrous particles, then you need do x-ray

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analysis only on those particles that satisfy your size and shape criteria.

The three-component diagrams, cited frequently by minerologists, are not really adequate, for distinguishing particles on the basis of chemistry because we are dealing with minerals with more than three variable components. A more general approach is the use of a decision tree (Fig. 1) in which is set up at each node a linear discriminant to differentiate one set of particles from another. Proceeding downwards, one approaches the ends of the decision tree with a different mineral at each termination. The trouble with this approach is that the optimal decision tree may change with the kind of specimen one is looking at, and a decision cannot be made on this until one has all of the data.

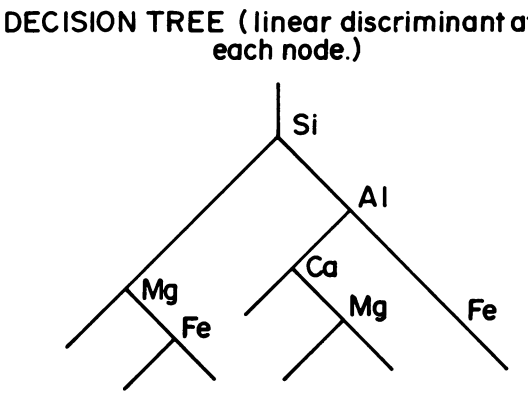

FIGURE 1. Decision tree (linear discriminant at each node). The optimal tree and discriminant functions may change depending on the specimen.

An alternative is to examine the specimens for two parameters at a time and plot the composition of the particles in the sample on a two-dimensional chart. In the example given in Figure 2, the two samples overlap in terms of the first pair of parameters, but not in terms of the second, so that they are clearly different minerals.

Finally, I must stress the importance of retaining samples and data for future reworking as new problems and new approaches develop.

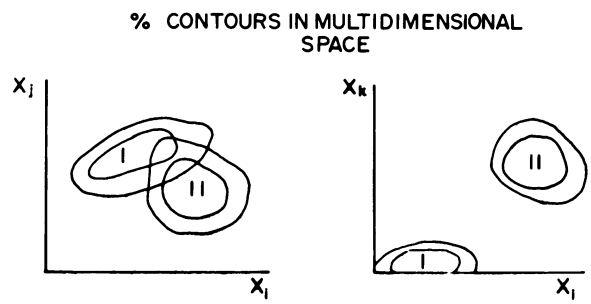

FIGURE 2. Contours in multidimensional space.